Blatt 9 - Hausaufgabe

Übung am 11. Januar 2019

Aufgabe 1: Direct correlation function

Find the direct correlation function of a homogeneous one-dimensional fluid of hard rods (length σ) knowing that the exact excess free energy functional is

$$\beta F_{\text{exc}}[\rho] = -\int dx \rho(x) \ln(1-\eta(x)), \tag{1}$$

where $\eta(x)$ is the local packing fraction:

$$\eta(x) = \int_x^{x+\sigma} dx' \rho(x'). \tag{2}$$

Aufgabe 2: A WDA functional for hard spheres

(a) Let $p(\rho)$ be the bulk equation of state of a given system. Show that the corresponding Helmholtz free energy per particle is:

$$\frac{F}{N} = \int_0^\eta \frac{p}{\rho\eta'} d\eta', \tag{3}$$

where η is the packing fraction.

(b) The approximate Carnahan-Starling bulk equation of state for hard spheres is

$$\frac{\beta p}{\rho} = \frac{1+\eta+\eta^2-\eta^3}{(1-\eta)^3}, \tag{4}$$

where $\eta = \pi/6\sigma^3\rho$ is the packing fraction of hard spheres of diameter σ. Use the above results to construct an approximated weighted density functional (WDA) for hard spheres (use a normalized step function of range σ as a weight function).

(c) Apply the same concepts to construct a WDA functional for the one-dimensional fluid of hard rods.

Blatt 9 - Präsenzübung

Übung am 11. Januar 2019

Aufgabe 3: Second virial coefficient

a) Calculate the second order contribution to the virial series in a homogeneous system of hard spheres.

Consider a two-dimensional system of hard line segments of length L.

b) Calculate the excluded area between two line segments at an arbitrary relative orientation (the excluded area is the region in which a particle cannot be located due to the presence of another particle at the origin).

c) The density distribution of the system can be written as $\rho(\mathbf{r}, \phi) = \rho(\mathbf{r})f(\mathbf{r}, \phi)$, with $f(\mathbf{r}, \phi)$ the orientational distribution function at position $\mathbf{r}$. Using the previous result write down a functional for a spatially homogeneous system of line segments based on the second order virial coefficient.